Incompressible excitonic superfluid of ultracold Bose atoms in an optical lattice: a new superfluid phase in the one-component Bose-Hubbard model

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We predict that a new superfluid phase, the incompressible excitonic superfluid (IESF), in the phase diagram of ultracold Bose atoms in $d > 1$ dimensional optical lattices, which is caused by the spontaneous breaking of the symmetry of translation of the lattice. Within mean field theory, the critical temperature of the phase transition from this IESF to the normal fluid (NF) is calculated and the triple-critical point of the three phases is determined. We also investigate both configuration and gauge field fluctuations and show the IESF state is stable against these fluctuations. We expect this IESF phase can be experimentally observed by loading cold Bose atoms into a two-dimensional lattice where the atom filling fraction deviates slightly from exact commensurations. The signatures distinguishing this IESF from the common atom superfluid (ASF) are that (i) the critical temperature of the IEST/NF transition is independent of interaction, unlike the ASF/NF transition; (ii) the IESF is incompressible while the ASF is compressible.

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Ultracold atoms in optical lattices offer new opportunities to study strongly correlated phenomena in a highly controllable environment[1, 2, 3, 4]. A quantum phase transition, the superfluid/Mott-insulator transition, was demonstrated using ^{87}Rb atoms [2, 4]. Strongly correlated phenomena for boson systems may be studied theoretically by the Bose-Hubbard model [5, 6]. Most studies focused on the quantum phase transition from the superfluid to the Mott insulator for a commensurate lattice at zero temperature.

Recently, the phase diagram of the ultracold Bose atoms has been investigated by Dickerscheid et al [7] by a slave boson approach and greatly improved by a slave fermion approach [8]. It was claimed that the Mott insulator phase crossovers to the normal fluid (NF) in a finite temperature for a commensurate lattice. For an incommensurate lattice, it was believed that below a critical temperature, the atoms are in the superfluid phase even in the strong interaction limit if the normal state is thought as a NF. To our knowledge, the phase structure of the normal state has not been thoroughly analyzed.

We define the 'normal' state of the one-component ultracold bose atoms in $d > 1$ optical lattices by the vanishing of the order parameter of the common atom superfluid(ASF). We find that there is an incompressible (atom-hole) excitonic superfluid (IESF) phase, due to the spontaneous breaking of the symmetry of translation of the lattice. For the commensurate filling fraction, this IESF phase is right above the zero temperature Mott insulator. Moreover, for an integer filling fraction, creating an atom-hole pair is accompanied by a double occupation. Thus, the IESF phase is enshrouded by the crossover from the Mott insulator to NL. To observe this IESF phase, the atom filling fraction of the lattice has to be incommensurate. As we will see that the critical temperature of the NF/IESF transition is very low. If the filling fraction deviates from the commensuration, say one percent from the one atom per site, the critical temperature of the NF/ASF transition will be higher than the critical temperature of the NF/IESF transition for a quite strong interacting strength. Thus, to observe such an IESF state, the filling fraction has to be not exact but very close to an integer. The justification to distinguish this IESF from the ASF is that the critical temperature of the IESF/NF transition is not interacting-dependent while the critical temperature of the ASF/NF transition decreases as the interaction strength increases. On the other hand, the IESF is incompressible while the ASF is compressible.

We investigate the ultracold atoms by the Bose-Hubbard model [5, 6] with Hamiltonian $H = -t\sum_{\langle ij\rangle} a_i^\dagger a_j - \mu\sum n_i + \frac{U}{2}\sum_i n_i(n_i-1) + V_{trap}$. Here $a_i^\dagger$ is a Bose atom creating operator on site i and the symbol $\langle ij\rangle$ denotes the sum over all nearest neighbor sites. μ is the chemical potential. t is the hopping amplitude and U the on-site interaction, which are determined by the optical lattice parameters and the s-wave scattering length of the atoms. We study $d > 1$ optical lattices only in this work. We first consider a homogeneous case with $V_{trap} = 0$. In order to explore the finite temperature behavior, we decompose the boson operator by the slave fermions, $a_i^\dagger = \sum_{\alpha=0}^{\infty}\sqrt{\alpha+1}c^\dagger_{\alpha+1,i}c_{\alpha,i}$, where the slave fermion operators $c_{\alpha,i}$ obey $\{c_{\alpha,i}, c^\dagger_{\beta,j}\} = \delta_{\alpha\beta}\delta_{ij}$. As the auxiliary particles, they have to obey the constraint $\sum_\alpha n_i^\alpha = \sum_\alpha c^\dagger_{\alpha,i}c_{\alpha,i} = 1$ on each site. In the slave fermion language, the partition function of the system reads $Z = \mathrm{Tr}e^{-\beta H} = \int Dc_\alpha Dc^\dagger_\alpha D\lambda\, e^{-S_E}$ where [8]

$$\begin{aligned} S_E[\bar{c}_\alpha, c_\alpha, \lambda] = \int_0^{1/T} d\tau \Big\{ \sum_i\sum_\alpha c^\dagger_{\alpha,i}[\partial_\tau - \mu \\ + \frac{U}{2}\alpha(\alpha-1) + i\lambda_i]c_{\alpha,i} - i\sum_i \lambda_i \\ - t\sum_{\langle ij\rangle}\sum_{\alpha\beta}\sqrt{\alpha+1}\sqrt{\beta+1}c^\dagger_{\alpha+1,i}c_{\alpha,i}c^\dagger_{\beta,j}c_{\beta+1,j} \Big\}, \end{aligned} \quad (1)$$

where λ_i is a Lagrange multiplier field and n is the atom filling fraction of the lattice.

To study the ASF/NL transition, we decouple the four slave fermion term by introducing a Hubbard-Stratonovich field Φ_i, which is a bosonic field and may be identified as the order parameter of the common atom superfluid. In our recent work, we have given the details to describe this phase transition by the slave fermion approach [8]. We find that using a finite type slave fermion approximation, say the maximal $\alpha_M = 6$, the well-known special points in the phase diagram may be well reproduced [9]. For example, for the filling fraction $n = 1$, the non-interacting Bose gas in a three-dimensional lattice has the critical temperature $T_c \approx 7.08t$ while our calculation for $\alpha_M = 6$ gives $T_c \approx 7.01t$; the zero temperature critical interacting strength from the superfluid to Mott insulator is $U_c/zt \approx 5.82$ in the mean field theory [10] while our result is $U_c/zt \approx 5.9$.

We now focus on the 'normal' state in which $\langle\Phi_i\rangle = 0$. We decompose the four slave fermion term by auxiliary Hubbard-Stratonovich fields $\hat\chi_{\alpha\beta,ij}$ and $\hat\eta_{\alpha\beta,ij}$, namely, the Lagrangian of the system is rewritten as

$$\begin{aligned} L &= \sum_i\sum_\alpha c^\dagger_{\alpha i}[\partial_\tau - \alpha\mu + \frac{U}{2}\alpha(\alpha-1) - i\lambda_i]c_{\alpha i} \\ &+ i\sum_i \lambda_i + \frac{1}{2}\sum_{\langle ij\rangle}\sum_{\alpha\beta} t_{\alpha\beta}[\hat\chi^\dagger_{\alpha\beta,ij}\hat\chi_{\alpha+1\beta+1,ij} \\ &- \hat\eta^\dagger_{\alpha\beta,ij}(\hat\chi_{\alpha+1\beta+1,ij} - c^\dagger_{\alpha+1,i}c_{\beta+1,j}) + h.c.], \end{aligned} \quad (2)$$

where $t_{\alpha\beta} = t\sqrt{\alpha+1}\sqrt{\beta+1}$. Integrating over $\hat\eta$ and $\hat\chi$, the above Lagrangian restores the original one. The auxiliary fields $\hat\chi_{\alpha\beta,ij}$, $\hat\eta_{\alpha\beta,ij}$ and λ_i may be rewritten as $\hat\chi_{\alpha\beta,ij} = \chi_{\alpha\beta,ij}e^{i\mathcal{A}_{ij}}$, $\hat\eta_{\alpha\beta,ij} = \eta_{\alpha\beta,ij}e^{i\mathcal{A}_{ij}}$ and $\lambda_i = \lambda + \mathcal{A}_{i0}$. Consider the mean field state, $\hat\chi_{\alpha\beta,ij} \approx \chi_{\alpha,ij}\delta_{\alpha\beta}$, $\hat\eta_{\alpha\beta,ij} \approx \eta_{\alpha,ij}\delta_{\alpha\beta}$, and $\lambda_i \approx \lambda$. The mean field Lagrangian reads

$$\begin{aligned} L_{MF} &= \sum_{i,\alpha} c^\dagger_{\alpha i}M_\alpha c_{\alpha i} - \sum_{\langle ij\rangle}\sum_\alpha \frac{1}{2}[t_\alpha(\eta^\dagger_{\alpha,ij} - \chi^\dagger_{\alpha,ij})\chi_{\alpha+1,ij} \\ &- (t_{\alpha-1}\eta^\dagger_{\alpha-1,ij} + t_\alpha\eta_{\alpha+1,ji})c^\dagger_{\alpha i}c_{\alpha j} + h.c.], \end{aligned} \quad (3)$$

where $M_\alpha = \partial_\tau - \alpha\mu + \frac{U}{2}\alpha(\alpha-1) - i\lambda$. The free single slave fermion Green's functions can be read out from (3),i.e., $\hat D_\alpha(x,\tau) = T\sum_n e^{i\omega_n\tau}\hat D_\alpha(\omega_n)$ with the matrix

$$\begin{aligned} \hat D_\alpha(\omega_n) &= [(i\omega_n + \frac{U}{2}\alpha(\alpha-1) - \mu + i\lambda)\delta_{ij} \\ &+ t_{\alpha-1}\eta^\dagger_{\alpha-1,ij} + t_\alpha\eta_{\alpha+1,ji}]^{-1}. \end{aligned} \quad (4)$$

The mean field equations are given by $\chi_{\alpha,ij} = \eta_{\alpha,ij}$ and $\eta_{\alpha,ij} = \langle c^\dagger_{\alpha i}c_{\alpha j}\rangle = T\sum_n D_{ij,\alpha}(\omega_n)$. Near the critical temperature, these mean field equations have the following solutions

$$\eta_{\alpha,ij}T_c^{(\alpha)} = \frac{t_{\alpha-1}\eta^\dagger_{\alpha-1,ij} + t_\alpha\eta^\dagger_{\alpha+1,ij}}{(e^{\beta_c^{(\alpha)}(\frac{U}{2}\alpha(\alpha-1)-\alpha\mu-i\lambda)}+1)^2}. \quad (5)$$

For $\alpha \geq 2$, the critical temperatures vanish, $T_c^{(\alpha)} = 0$, while

$$T_c^{(0)} = \frac{\eta_1^\dagger}{4\eta_0}t, \qquad T_c^{(1)} \approx \frac{\eta_0^\dagger}{\eta_1}t, \quad (6)$$

if $\beta_c\mu \gg 1$. The coupling between η_0 and η_1 means $\eta_1 = 2\eta_0^\dagger$ and $T_c^{(0)} = T_c^{(1)} = T_c = t/2$ [11]. Changing the variable $\Delta_0 = -i\eta_0/t$ and using $\eta_1 = 2\eta_0^\dagger$, the mean field free energy near the critical temperature may be expanded by [12]

$$\begin{aligned} F &= \sum_{\langle ij\rangle}(2t^{-1}\Delta^2_{0,ij} - T^{-1}|\Delta_{0,ij}|^2) \\ &+ \frac{1}{24T_c^3}\sum_{\langle ijkl\rangle}\Delta_{0,ij}\Delta_{0,jk}\Delta_{0,kl}\Delta_{0,li}. \end{aligned} \quad (7)$$

The first term in (7) implies only a real $\Delta_{0,ij}$ minimizes the free energy, which is given by

$$F = -3t\tau^2 S_2^2/S_4, \quad (8)$$

where $\tau = \frac{T_c - T}{T}$; S_2 and S_4 are the numbers of the non-zero terms of the first and second summations in (7). Due to the filling fraction very close to $n = 1$, we consider all holes in the lattice are isolated. There are two solutions. One is the equal-bond state. Namely, for a hole at site i, $\Delta_{0,i,i\pm\tau_x} = -\Delta_{0,i,i\pm\tau_y} = \Delta_0$ for all nearest neighbor sites j and all others are zero. Another solution is an atom-hole exciton state and $\Delta_{0,ij} = \Delta_0$ is not zero only if a link (ij) is occupied by an exciton, *which breaks the symmetry of translation of the lattice in the link direction.* The free energies per site for the equal-bond and exciton states are degenerate, e.g., for a two-dimensional square lattice with a low hole density,

$$f_{eb} = f_e = -6n^0 t\tau^2, \quad (9)$$

where n^0 is the hole density. There is, however, a configuration fluctuation to the equal-bond state. When two holes are close so that they are in the diagonal line of a plaquette, the equal-bond state will gain the free energy an amount $\frac{4}{3}t\tau^2$ while the free energy of the exciton state does not change. Multi-hole configurations further raise the energy of the equal-bond state. On the other hand, due to the gauge fluctuation as we shall see the equal-bond state may not be stable.

To study the gauge fluctuations, we first calculate the dispersion relations of the slave fermions for these two mean field states. For a two-dimensional square lattice, we divide the lattice into two sublattices, even and odd. The slave fermion operators $c_{\alpha,i}$ is denoted by either $e_{\alpha,i}$ or $d_{\alpha,i}$, corresponding to $i \in$ even or odd, respectively. Using the Fourier components $e_{\alpha,k} = \frac{1}{\sqrt{N/2}}\sum_{i\in even}e^{-ik\cdot R_i}e_{\alpha,i}$ and $d_{\alpha,k} = \frac{1}{\sqrt{N/2}}\sum_{i\in odd}e^{-ik\cdot R_i}d_{\alpha,i}$, the hopping term of the Hamiltonian in the mean field theory may be diagonalized

$$H_t = \sum_{\alpha=0,1;k}|\Delta^{(\alpha)}(k)|(\zeta^\dagger_{\alpha,k}\zeta_{\alpha,k} - \xi^\dagger_{\alpha,k}\xi_{\alpha,k}), \quad (10)$$

where $\Delta^{(0)}(k) = \Delta_1(k)$ and $\Delta^{(1)}(k) = \Delta_0(k)$. $\Delta_\alpha(k) = \Delta_{\alpha,1}e^{ik_x} - \Delta_{\alpha,2}e^{-ik_y} + \Delta_{\alpha,3}e^{-ik_x} - \Delta_{\alpha,4}e^{ik_y}$ where 1,2,3 and 4 denote four adjacent sites around a hole. The diagonalized operators are defined by

$$e_{\alpha,k} = \sqrt{\frac{1}{2}}(\xi_{\alpha,k} + \frac{i\Delta^*_{\alpha,k}}{|\Delta_{\alpha,k}|}\zeta_{\alpha,k}),$$
$$d_{\alpha,k} = \sqrt{\frac{1}{2}}(-\frac{i\Delta^*_{\alpha,k}}{|\Delta_{\alpha,k}|}\xi_{\alpha,k} + \zeta_{\alpha,k}). \quad (11)$$

For the equal-bond state, the slave fermion dispersions are $\epsilon_{eb,\alpha}(k) = \pm 2|\Delta_\alpha|(\cos k_x + \cos k_y)$, which have gapless excitations. For the exciton, the slave quasi-fermions are dispersionless with $\epsilon_{d,\alpha}(k) = \pm|\Delta_\alpha|$, which means that exciting a slave quasi-fermion has an energy gap $|\Delta_\alpha|$. However, the slave fermions are auxiliary particles and the single slave fermion Green's function is not gauge invariant. To see the real quasiparticle excitation, one has to calculate a gauge invariant Green's function. The single-atom thermodynamic Green's function is gauge invariant, which reads

$$\langle T(a(x,t)a^\dagger(0,0))\rangle = \sum_{\alpha\beta}\sqrt{\alpha+1}\sqrt{\beta+1}$$
$$\langle T(c^\dagger_\alpha(x,t)c_{\alpha+1}(x,t)c^\dagger_{\beta+1}(0,0)c_\beta(0,0))\rangle. \quad (12)$$

If we consider the lowest lying excitation, only relevant propagating processes are those which do not raise an additional on-site energy U. That is, at $t = 0$, positions x and 0 have the occupation numbers α and $\alpha+1$, respectively, and after a time t, one atom propagates from 0 to x, the occupation numbers become $\alpha+1$ at x and α at 0. The approximation we are using yields the following factorization of the four slave fermion Green's function, $\sum_{\alpha\beta}\sqrt{\alpha+1}\sqrt{\beta+1}\langle T(c^\dagger_\alpha(x,t)c_{\alpha+1}(x,\tau)c^\dagger_{\beta+1}(0,0)c_\beta(0,0))\rangle \approx \sum_\alpha(\alpha+1)\langle T(c^\dagger_\alpha(x,t)c_\alpha(0,0))\rangle\langle T(c_{\alpha+1}(x,t)c^\dagger_{\alpha+1}(0,0))\rangle$. The corresponding retarded Green's function is given by

$$G^R(\omega) \propto \sum_\alpha \frac{(\alpha+1)(n^\alpha - n^{\alpha+1})}{\omega - \alpha U + |\Delta^{(\alpha+1)}| - |\Delta^{(\alpha)}| + \mu + i0^+} \quad (13)$$

where the order parameters $\Delta^{(0)} = \Delta_1$, $\Delta^{(1)} = \Delta_0$ and vanish for others.

Thus, the lowest energy quasiparticle excitation at finite temperature is

$$\varepsilon(k) = |\Delta_1(k)| - |\Delta_0(k)| = |\Delta_0(k)|. \quad (14)$$

This implies the low lying excitations of the exciton state has a gap $|\Delta_0|$, which is equal to t at $T = 0$, while it is gapless for the equal-bond state. The second level excitation spends an energy $U - |\Delta_1(k)|$.

We now discuss the gauge fluctuations. The gauge fluctuations come from the gauge field $\mathcal{A}_{ij}$ and $\mathcal{A}_{0i}$. For the equal-bond state, the gauge fluctuations may be more serious than in the t-J model because we do not have a large N limit. However, the existence of the gap in

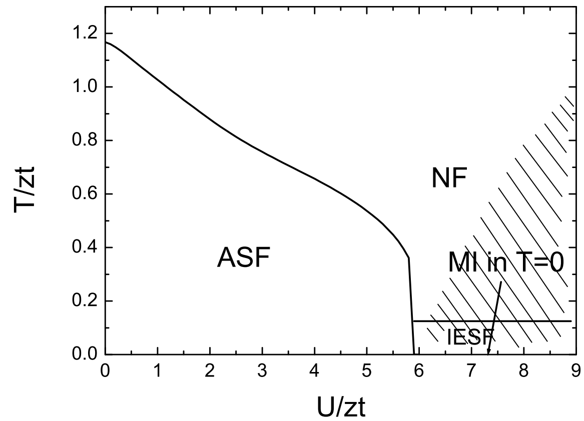

FIG. 1: The phase diagram for 2d for n=1. ASF, NF, IESF and MI are standing for the atom superfluid, normal fluid, incompressible excitonic superfluid and Mott insulator, respectively. The shadowed area is the crossover regime from MI to NF.

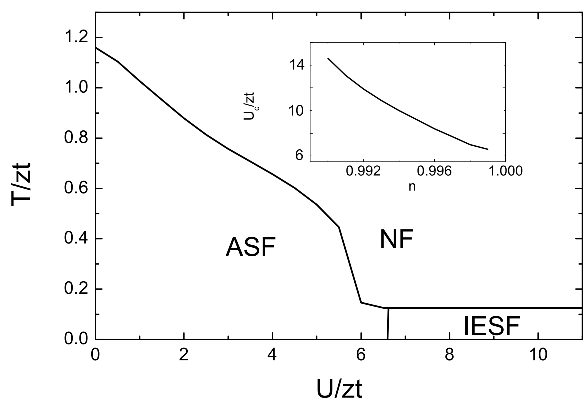

FIG. 2: the phase diagram for 2d for n=0.999. The inset is the value of U_c in the triple-critical varying as the atom filling fraction.

the exciton state strongly suppresses the gauge fluctuations. Integral over the slave fermion field, one can get the effective action of the gauge field

$$S[a] = \frac{T}{2}\int d^2k a_\mu(k,\omega)a_\nu(k,\omega)\Pi_{\mu\nu}(k,\omega),$$
$$\Pi_{\mu\nu} = \sum_\alpha \int d^2p\Big[\frac{n^\alpha(p+k/2) - n^\alpha(p-k/2)}{\omega - [\epsilon_\alpha(p+k/2) - \epsilon_\alpha(p-k/2)]}$$
$$\times\frac{\partial\epsilon_\alpha}{\partial p_\mu}\frac{\partial\epsilon_\alpha}{\partial p_\nu} + \frac{\partial^2\epsilon_\alpha}{\partial p_\mu\partial p_\nu}n(p)\Big], \quad (15)$$

where $a_\mu(k,\omega)$ is the Fourier component of the continuum limit of the gauge field. The dispersionless of

the exciton state means $\Pi_{\mu\nu} = 0$ which suppresses the gauge fluctuation. The physical meaning of $\Pi_{\mu\nu}$ is the atom density-density and current-current correlation functions. The vanishing of the density-density correlation function yields the incompressibility of the state.

For the equal-bond state, the gauge field propagator $\Pi^{-1}_{\mu\nu} = \langle a_\mu(q)a_\nu(-q)\rangle = (\delta_{\mu\nu} - q_\mu q_\nu/q^2)D_T(\vec{q})$ with $D_T(\vec{q}) \simeq [i\omega/q - \chi_d q^2]^{-1}$ for $\omega < q$ [13]. The gauge fluctuation may renormalize the hopping amplitude t to $\tilde{t} = t\langle e^{i\mathcal{A}_{ij}}\rangle = te^{-\langle\mathcal{A}^2_{ij}\rangle}$ and the critical temperature is reduced to $\tilde{T}_c = \tilde{t}/2$.

To sum up, both configuration and gauge fluctuations destroy the equal-bond state while the exciton state is safe. The excitons form an incompressible fluid. Furthermore, because $\Delta_1 = 2\Delta_0 \neq 0$, the order parameter $\langle a^\dagger_i a_j\rangle$ of the exciton condensate is not zero. This means the excitons are condensed when $T < T_c$. This is an incompressible excitonic superfluid (IESF).

The phase diagrams of the system now may be depicted according to the above discussions. Fig.1 is the phase diagram for the filling fraction $n = 1$ for two-dimensions. There is a triple-critical point with $U_c/zt \approx 5.8$ and $T_c/zt = 1/2z$. The IESF is right above the Mott insulator. Therefore, this IESF may not be observed in the commensurate filling fraction because the IESF is still in the range of the practical Mott insulator. The crossover from the Mott insulator to the normal fluid enshrouds this IESF phase. To observe the IESF phase, one should work in an incommensurate filling fraction. However, the critical temperature $T_c = t/2$ is so low that the $U_c/zt \sim 15$ for $n = 0.99$ in two-dimensions. In the inset of Fig. 2, we show the critical U_c for $0.99 \leq n \leq 0.999$. Thus, the IESF can only be observed when the filling fraction deviates slightly from the commensuration. In Fig. 2, we show the phase diagram for $n = 0.999$ for two dimensions. For three dimensions, the triple-critical point is $U_c/zt \sim 16$ for $n = 0.999$, much stronger than that in two dimensions.

We now briefly discuss the inhomogeneous case with a trap potential $V_{trap} = V\sum_i r_i^2 n_i$ where r_i is the distance of an atom from the center of the trap. In the regime of U we are concerning, there is a central Mott plateau which is surrounded by a superfluid ring [14]. Our result points out that there, in fact, are two superfluid rings. The IESF ring right surrounds the Mott plateau and the ASF ring is outside of the IESF ring. As U is enhanced, while the radius of the Mott plateau almost will not vary, the radius of the zero compressibility valley will be enlarged because the IESF ring becomes wider. This requires an examination by a quantum Monte Carlo calculation, which will be reported elsewhere because it will take a long computing time period and more space to describe.

In conclusion, we predicted a new superfluid phase, the incompressible excitonic superfluid, in the one-component Bose-Hubbard model for $d > 1$ if the on-site interaction is large enough. This may be observed when the atom filling fraction deviates slightly from a commensurate one. Two characteristics of the IESF may be distinguished from the atom superfluid: (i) the incompressibility of the IESF with a gap $\sim 0.1\mu$K at $T = 0$ for ^{87}Rb (The Mott gap $> 2.5\mu$K.); and (ii) the U-independence of the critical temperature $T_c = t/2 \sim 0.05\mu$K. We calculated the free energy in a mean field theory and analyzed the configuration and quantum fluctuations. We intend to examine this IESF phase by a quantum Monte Carlo calculation.

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